



chain nodes :  
 16 17 18 19 20 21 22 23 39 40 41 42 43 44 45 46 47 48 49  
 ring nodes :  
 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 24 25 26 27 28 29 30 31 32 33 34  
 35 36 37 38  
 chain bonds :  
 2-22 3-21 4-20 9-16 14-23 16-17 17-18 17-19 25-45 26-44 27-43 32-39 37-46 39-40  
 40-41 40-42 46-47 46-48 47-49  
 ring bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-11 7-8 7-12 8-9 8-15 9-10 10-11 12-13 13-14 14-15  
 24-25 24-29 25-26 26-27 27-28 28-29 28-30 29-34 30-31 30-35 31-32 31-38 32-33  
 33-34 35-36 36-37 37-38  
 exact/norm bonds :  
 9-16 14-23 16-17 17-19 32-39 39-40 40-42 46-47 46-48 47-49  
 exact bonds :  
 2-22 3-21 4-20 5-7 6-11 8-9 9-10 10-11 17-18 25-45 26-44 27-43 28-30 29-34 31-32  
 32-33 33-34 37-46 40-41  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-15 12-13 13-14 14-15 24-25 24-29 25-26 26-27  
 27-28 28-29 30-31 30-35 31-38 35-36 36-37 37-38  
 isolated ring systems :  
 containing 1 : 24 :

G1:H,Ph,Cb,Ak

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS  
 22:CLASS 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom  
 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:CLASS 40:CLASS 41:CLASS  
 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS  
 fragments assigned product role:  
 containing 1  
 fragments assigned reactant/reagent role:

containing 24